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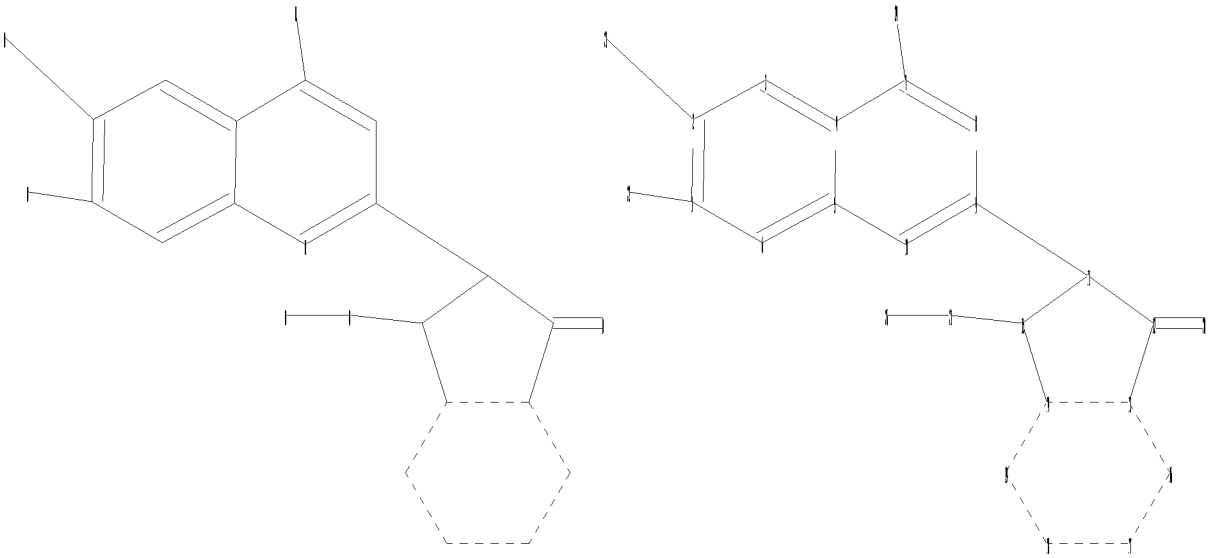
FILE 'HOME' ENTERED AT 10:02:19 ON 11 FEB 2009

=> file reg

=>
Uploading C:\Program Files\Stnexp\Queries\11560039.str

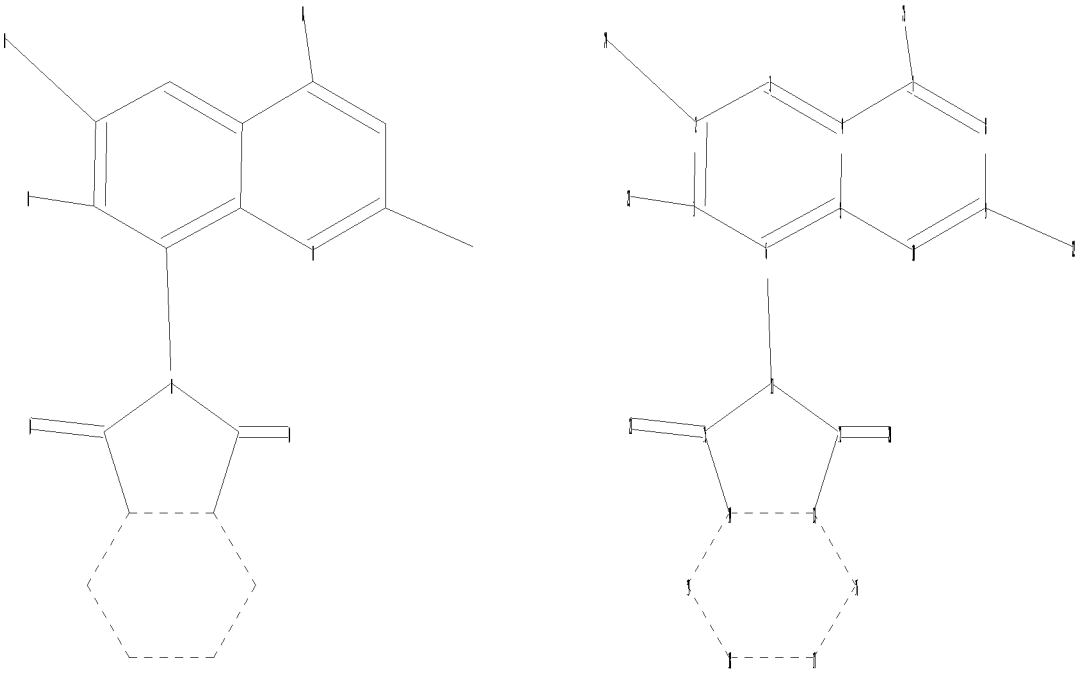


chain nodes :
20 21 22 23 24 26
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
chain bonds :
1-22 2-23 7-24 9-11 12-20 15-21 21-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 11-15 11-12 12-13 13-14
 13-16 14-15 14-19 16-17 17-18 18-19
exact/norm bonds :
11-15 11-12 12-13 12-20 13-14 13-16 14-15 14-19 15-21 16-17 17-18 18-19
exact bonds :
1-22 2-23 7-24 9-11 21-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\10560039.str

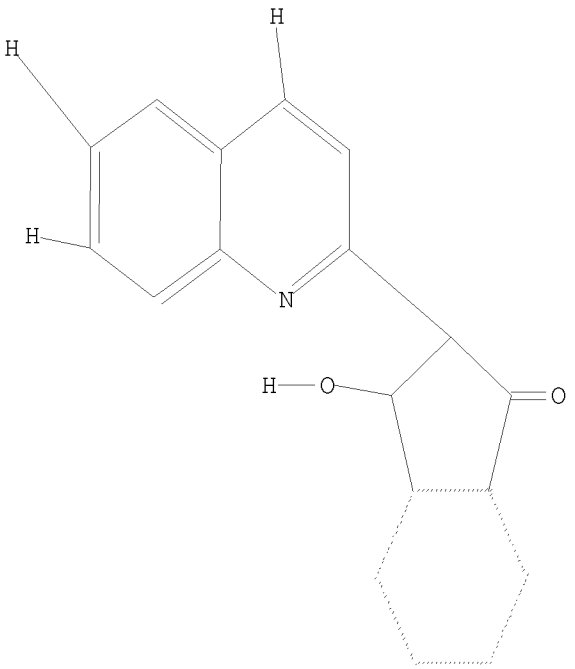


chain nodes :
20 21 22 23 24 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
chain bonds :
1-23 2-24 6-11 7-25 9-22 12-20 15-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14
13-16 14-15 14-19 16-17 17-18 18-19
exact/norm bonds :
6-11 11-12 11-15 12-13 12-20 13-14 13-16 14-15 14-19 15-21 16-17 17-18
18-19
exact bonds :
1-23 2-24 7-25 9-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

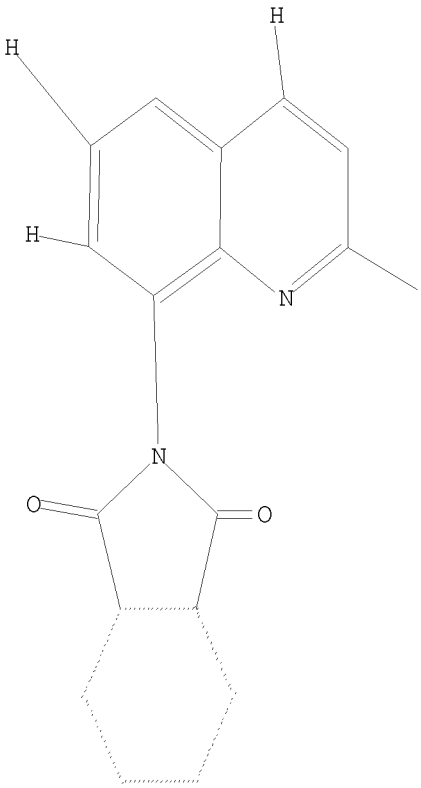
L2 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> d l2
L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

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=> s l1 full
FULL SEARCH INITIATED 10:03:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2343 TO ITERATE

100.0% PROCESSED     2343 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

L5            2 SEA SSS FUL L1

=> s l2 full
FULL SEARCH INITIATED 10:03:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      287 TO ITERATE

100.0% PROCESSED      287 ITERATIONS                                12 ANSWERS
SEARCH TIME: 00.00.01

L6           12 SEA SSS FUL L2

=> file ca

=> s l5 or l6
             2 L5
```

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             6 L6
L7           8 L5 OR L6

=> d ibib abs fhitstr 1-8

L7   ANSWER 1 OF 8  CA  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        142:58225  CA
TITLE:                   Use of quinaldine and naphthalene derivatives as
                         crystallization modifiers for quinophthalone (and
                         other) pigments.
INVENTOR(S):             Stohr, Andreas; Schroeck, Manfred
PATENT ASSIGNEE(S):      BASF Aktiengesellschaft, Germany
SOURCE:                  PCT Int. Appl., 33 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                German
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     ---------------     ----   --------    --------------------    --------
     WO 2004108837        A1    20041216    WO 2004-EP6164          20040608
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     DE 10326631          A1    20050105    DE 2003-10326631        20030611
     TW 258496            B     20060721    TW 2004-93113356        20040512
     EP 1641885           A1    20060405    EP 2004-739693          20040608
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
     CN 1806016           A     20060719    CN 2004-80016427        20040608
     JP 2006527290        T     20061130    JP 2006-515849          20040608
     US 20060150866       A1    20060713    US 2005-560039          20051208
PRIORITY APPLN. INFO.:                       DE 2003-10326631    A   20030611
                                             WO 2004-EP6164      W   20040608

OTHER SOURCE(S):         MARPAT 142:58225
GI
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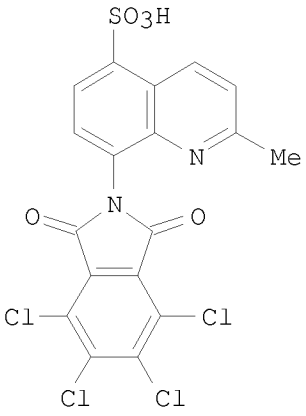


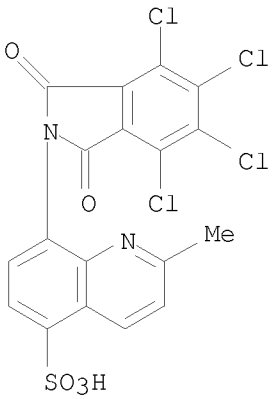
I

AB Quinaldine and naphthalene derivs. are useful as crystallization modifiers in the process of grinding and recrystn. of crude quinophthalone pigments from aqueous or/and organic solvent/water mixts. into fine-particle pigments. Thus, I (prepared by heating a mixture containing 100 g of phenol, 34 g of 8-aminoquinaldine-5-sulfonic acid and 49 g of tetrachlorophthalic anhydride 8 h at 180°, cooling to 90°, adding 300 mL of methanol, washing and drying at 40°) is used in recrystn. of crude quinophthalone pigment having particle size 2 cm (Pigment yellow 138) from xylene solution with additives of aliphatic amines.

IT 807657-04-1P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(crystallization modifier; quinaldine and naphthalene derivs. as crystallization modifiers in grinding and recrystn. of crude quinophthalone pigments)

RN 807657-04-1 CA

CN 5-Quinolinesulfonic acid, 2-methyl-8-(4,5,6,7-tetrachloro-1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)- (CA INDEX NAME)

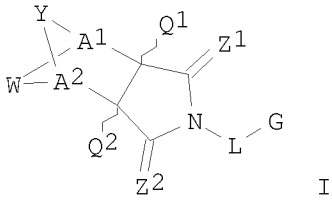


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 8 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 137:216934 CA
TITLE: Preparation of fused cyclic succinimide compounds and analogs thereof, as modulators of nuclear hormone receptor function
INVENTOR(S): Salvati, Mark E.; Attar, Ricardo M.; Gottardis, Marco M.; Balog, James A.; Pickering, Dacia A.; Martinez, Rogelio L.; Sun, Chongqing
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 331 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002067939	A1	20020906	WO 2002-US5302		20020220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
US 20040087548	A1	20040506	US 2002-75870		20020214
CA 2439265	A1	20020906	CA 2002-2439265		20020220
AU 2002250163	A1	20020912	AU 2002-250163		20020220
EP 1379249	A1	20040114	EP 2002-719057		20020220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
HU 2003004055	A2	20040428	HU 2003-4055		20020220
JP 2004523558	T	20040805	JP 2002-567306		20020220
US 20060111424	A1	20060525	US 2005-311731		20051219
PRIORITY APPLN. INFO.:			US 2001-271672P	P	20010227
			US 2002-75870	A1	20020214
			WO 2002-US5302	W	20020220

OTHER SOURCE(S): MARPAT 137:216934
GI



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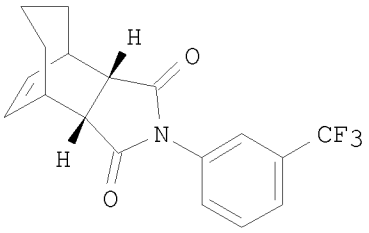


II

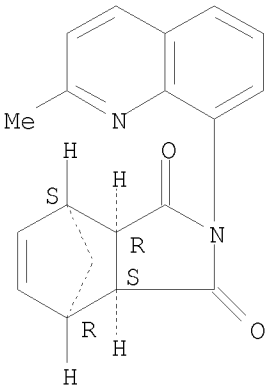
AB Title compds. I [G = (un)substituted cycloalkenyl, aryl or heterocyclo (mono or polycyclic); Z1 and Z2 independently = O, S, NH or substituted amine; L = bond, substituted alkyl chain, NH, substituted amine; A1 and A2 independently = CR1 or N when Y = J-J'-J'' where J = (CR1R1')n with n = 0-3, J' = bond, carbonyl, CR1R1', R2P:O, R2P:S, etc., and W = CR1R1'-CR1R1', CR3:CR3', (un)substituted cycloalkyl, etc.; or when Y is absent A1 and A2 independently = CR1R1' or NR1; or when Y is absent A1, A2 and W together form -NR1-N:N-; Q1 and Q2 independently = H, (un)substituted alkyl, alkenyl, cycloalkyl, etc.; R1 and R1' independently = H, (un)substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, amino, halo, CN, etc.; R2 = (un)substituted alkyl, cycloalkyl, cycloalkenyl, heterocyclo, aryl, arylalkyl, etc.; R3 and R3' independently = H, (un)substituted alkyl, alkenyl, CN, halo, nitro, amino, etc.] are prepared and methods of using such compds. in the treatment of nuclear hormone receptor-associated conditions, and pharmaceutical compns. containing such compds are disclosed. Thus, II was prepared by cyclocondensation of (3aα,4β,8β,8aα)-4,5,6,7,8,8a-hexahydro-4,8-etheno-1H-cyclohepta[c]furan-1,3(3aH)dione (preparation given) with 3-(trifluoromethyl)aniline. Combinatorial methods of preparing compds. of formula I are also provided. As modulators of nuclear hormone receptor function, the use of I as potential anticancer agents and for treatment of immune disorders is claimed (no data).

IT 455272-94-3P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(target compound; preparation of combinatorial libraries of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

RN 455272-94-3 CA

CN 4,7-Methano-1H-isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-(2-methyl-8-quinolinyl)-, (3aR,4S,7R,7aS)-rel- (CA INDEX NAME)

Relative stereochemistry.

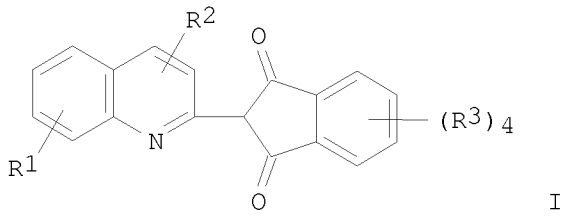


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

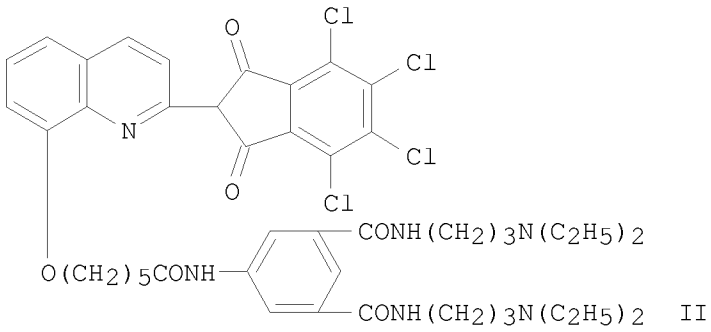
L7 ANSWER 3 OF 8 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 136:21013 CA
TITLE: Quinophthalone compounds, pigment dispersants therewith, their pigment dispersion compositions and colored photosensitive compositions
INVENTOR(S): Takeda, Akihiko; Sugiyama, Takekatsu; Kodama, Tomohiro
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001335711	A	20011204	JP 2000-159244	20000529
PRIORITY APPLN. INFO.:			JP 2000-159244	20000529

OTHER SOURCE(S): MARPAT 136:21013
GI



I



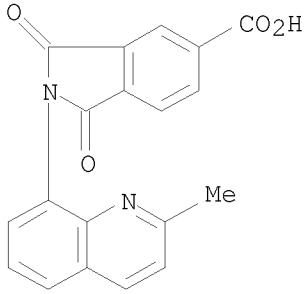
II

AB Title compds. show a structure as I [R1 = Q1Q2 and R2 = H, alkyl; or vice versa, Q1 = divalent group, Q2 = C6H5-a(XYZ)a, X = O, CONH, NHCO, COO, Y = low alkylene, Z = low alkylamino or N-containing 5-6 membered ring, a = 1-2; R3 = H, Cl]. A composition comprising C.I. pigment yellow 138 8.3, II [prepared from 8-hydroxy-2-methylquinoline, Et 6-bromohexanoate, bis(3-diethylaminopropylamido) 5-aminoisophthalate, and tetrachlorophthalic anhydride] 0.8, benzyl methacrylate-methacrylic acid copolymer 20.8, and 1-methoxy-2-Pr acetate 50.1 g showed viscosity 15 cP, which was used to prepare a photosensitive composition resulting high contrast value.

IT 377741-57-6P
RL: CRT (Combinatorial reactant); IMF (Industrial manufacture); RCT (Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of quinophthalone dispersants for pigment dispersion compns. for color filters)

RN 377741-57-6 CA

CN 1H-Isoindole-5-carboxylic acid, 2,3-dihydro-2-(2-methyl-8-quinolinyl)-1,3-dioxo- (CA INDEX NAME)



L7 ANSWER 4 OF 8 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 95:97579 CA
ORIGINAL REFERENCE NO.: 95:16387a,16390a
TITLE: Substituted anilines
INVENTOR(S): Schefczik, Ernst
PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2924066	A1	19801218	DE 1979-2924066	19790615
PRIORITY APPLN. INFO.:			DE 1979-2924066 A	19790615

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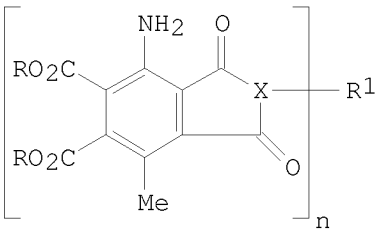

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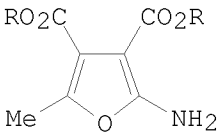


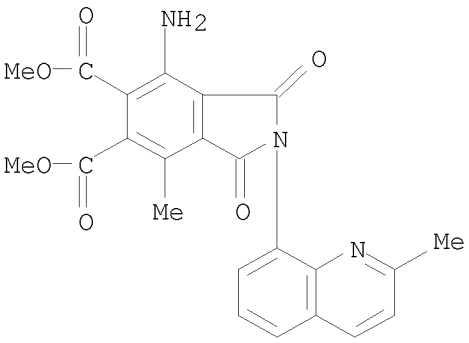
II

AB The title compds. [I; R = C1-8 alkyl; n = 1, X = O, XR1 = optionally substituted NH; n = 2, X = N, R1 = bond, divalent group] were prepared by the reaction of II with maleic anhydride (III) or a maleimide. Thus, II (R = Me) was heated with III in HOAc to give 94.5% I (R = Me, XR1 = O, n = 1). I are useful as diazo components or fluorescent agents.

IT 77554-64-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 77554-64-4 CA

CN 1H-Isoindole-5,6-dicarboxylic acid, 4-amino-2,3-dihydro-7-methyl-2-(2-methyl-8-quinolinyl)-1,3-dioxo-, 5,6-dimethyl ester (CA INDEX NAME)



L7 ANSWER 5 OF 8 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 87:7472 CA
ORIGINAL REFERENCE NO.: 87:1203a,1206a
TITLE: Coloring of polymers
INVENTOR(S): Shimada, Keizo; Harada, Toshiaki; Koga, Masahiro
PATENT ASSIGNEE(S): Teijin, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51147544	A	19761217	JP 1975-70752	19750613
JP 58012904	B	19830310		
DE 2626271	A1	19761223	DE 1976-2626271	19760611
DE 2626271	B2	19800911		
DE 2626271	C3	19810514		
CA 1078833	A1	19800603	CA 1976-254649	19760611
FR 2314226	A1	19770107	FR 1976-17926	19760614
FR 2314226	B1	19781117		

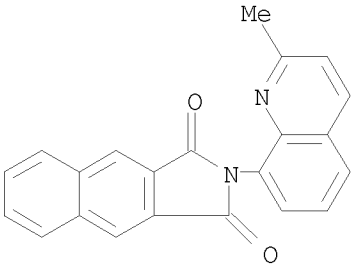
PRIORITY APPLN. INFO.: JP 1975-70220 A 19750612
JP 1975-70221 A 19750612
JP 1975-70752 A 19750613

GI

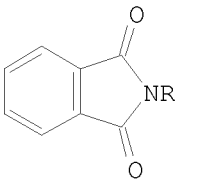
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Plastics and polyester fibers were colored yellow with I (R = Br, Cl; R1, R2 = H, Br) and II (R = H [61975-16-4], Br [61975-18-6]). For example, I (R = Cl, R1 = R2 = H) [61975-13-1] was prepared from 8-(2,3-naphthalenedicarboximido)quinaldine [62783-05-5] and tetrachlorophthalic anhydride [117-08-8] in the presence of ZnCl2, pelletized with polystyrene [9003-53-6] in 0.2:200 ratio at 230°, and injection-molded at 220-80° (dwelling time 2 min) to give a yellow molding with lightfastness rating >6.

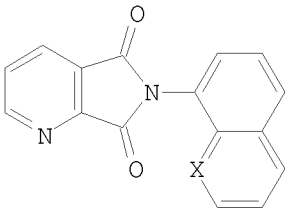
IT 62783-05-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tetrachlorophthalic anhydride)
RN 62783-05-5 CA
CN 1H-Benz[f]isoindole-1,3(2H)-dione, 2-(2-methyl-8-quinolinyl)- (CA INDEX NAME)



L7 ANSWER 6 OF 8 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 85:42101 CA
ORIGINAL REFERENCE NO.: 85:6835a,6838a
TITLE: Negative geotropic effect and phytotoxicity of N-quinolinephthalamic acids and related substances
AUTHOR(S): Pagani, G.; Caccialanza, G.
CORPORATE SOURCE: Dep. Chim. Farm., Univ. Pavia, Pavia, Italy
SOURCE: Farmaco, Edizione Scientifica (1976), 31(5), 364-71
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI



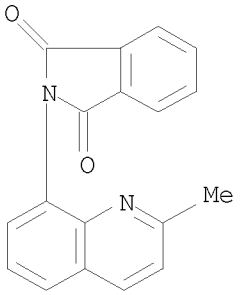
I



II, X=CH
III, X=N

AB Eleven N-phthalimidoquinolines I (R = quinolyl, methylquinolyl, methoxyquinolyl, etc.) were prepared and tested for neg. geotropic effect on Lens esculenta seedling roots, and for phytotoxic activity on 5 weed species. N-(2-quinolyl)phthalimide [49608-97-1], N-(8-quinolyl)phthalimide [19348-61-9], N-(2-methyl-8-quinolyl)phthalimide [59679-83-3] and N-(6-methoxy-8-quinolyl)phthalimide [59679-84-4] had the highest geotropic effect, which was identical to that of the standard N-(α-naphthyl)phthalimide. The 3 latter compds. showed the highest phytotoxic activity, especially when applied pre-emergence. II [37458-44-9] and III [59679-88-8], pyridine analogs of I, showed little activity.

IT 59679-83-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and herbicidal and geotropic activity of)
RN 59679-83-3 CA
CN 1H-Isoindole-1,3(2H)-dione, 2-(2-methyl-8-quinolinyl)- (CA INDEX NAME)



L7 ANSWER 7 OF 8 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 54:2349 CA
ORIGINAL REFERENCE NO.: 54:582f-i,583a-c
TITLE: Indenones substituted by quinolyl, pyridyl and benzimidazolyl radicals
INVENTOR(S): Amstutz, Edward D.; Krueger, Geraldine L.
PATENT ASSIGNEE(S): Wm. S. Merrell Co.
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2894952		19590714	US 1957-683214	19570911

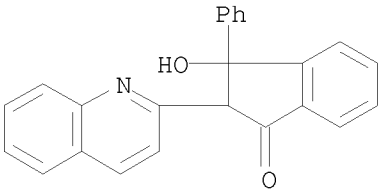
AB Certain 3-(R-substituted)-2-(Y-substituted)-1-indenones were prepared wherein R was a phenyl, lower alkyl phenyl, lower alkoxyphenyl or halophenyl radical and Y was a 2-pyridyl, 2-quinolyl, or 2-benzimidazolyl radical. By lower alkyl and lower alkoxy were meant groups containing 1 to 4 C atoms. Preferred halogens were Cl and Br. These compds. were used in treatment of inflammatory diseases such as rheumatoid arthritis, in the reversal of acute inflammatory lesions such as those of the eye, and for topical application on the skin and mucous membrane as in vaginitis. For oral or parenteral use dosage was 250 mg. to 1 g. daily. They could be a part of creams, ointments or lotions. For example, the intermediate 3-hydroxy-3-phenyl-2-(2-pyridyl)-1-indanone (I), was prepared by adding 0.94 g. Li filings in 50 cc. ether to a solution of 10.52 g. bromobenzene in 13 ml. ether under gentle reflux. After the mixture was cooled, 4.46 g. pyrophthalone was added during 0.5. hr. The solution was stirred 1 hr., refluxed 1 hr., water added and ether distilled during addition of 10% H2SO4 (acidification). A yellow solid was filtered off, washed with 10% H2SO4 and water and then washed with toluene. Crude product m. 134° (vigorous decomposition); after recrystn. from 95% EtOH it m. 142.2-2.8°. When I was heated until no yellow color remained, a red-orange solid, 3-phenyl-2-(2-pyridyl)-1-indenone (II), resulted. II recrystd. from 50% EtOH-H2O m. 129.8-30.8°; picrate m. 198-199.4°; oxime m. 185-6.5°. Similarly prepared were: the intermediate, 3-hydroxy-3-(p-methoxypheny)-2-(2-pyridyl)-1-indanone (III),

m. 159-60°; orange flakes of 3-(p-methoxyphenyl)-2-(2-pyridyl)-1-indenone (IV), m. 155.5-6.0°; the intermediate, 3-hydroxy-3-(p-tolyl)-2-(2-pyridyl)-1-indanone (V), m. 150-55°; bright red flakes of 3-(p-tolyl)-2-(2-pyridyl)-1-indenone (VI), m. 155-6°; the intermediate, a yellow solid, 3-hydroxy-3-(m-tolyl)-2-(2-pyridyl)-1-indanone (VII), m. 130-45°; an orange solid, 3-(m-tolyl)-2-(2-pyridyl)-1-indenone (VIII), m. 107-10°; the intermediate, a yellow solid, 3-hydroxy-3-(p-chlorophenyl)-2-(2-pyridyl)-1-indanone (IX), m. 150-60°; 3-(p-chlorophenyl)-2-(2-pyridyl)-1-indenone (X), m. 135.5-37.5°; the intermediate 3-hydroxy-3-phenyl-2-(2-quinolyl)-1-indanone (XI), a yellow solid, m. 182°; 3-phenyl-2-(2-quinolyl)-1-indenone-HCl (XII), orange crystals, m. 220-28°; the intermediate, a pale yellow solid, 3-hydroxy-3-phenyl-2-(2-benzimidazolyl)-1-indanone (XIII), m. 235°; 3-phenyl-2-(2-benzimidazolyl)-1-indenone (XIV), dark red, m. 255-57°. Methods were given for preparation of tablets, capsules, injectable suspensions, oral suspensions and ointments. The intermediate III also exhibited anti-inflammatory activity. It was useful orally, parenterally, and topically in dosages and uses described.

IT 102543-48-6P, 1-Indanone, 3-hydroxy-3-phenyl-2-(2-quinolyl)-
RL: PREP (Preparation)
(preparation of)

RN 102543-48-6 CA

CN 1H-Inden-1-one, 2,3-dihydro-3-hydroxy-3-phenyl-2-(2-quinolinyl)- (CA INDEX NAME)



L7 ANSWER 8 OF 8 CA COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 53:51147 CA

ORIGINAL REFERENCE NO.: 53:9210h-i,9211a-i,9212a-f

TITLE: Pyrophthalone and related compounds

AUTHOR(S): Manly, Donald G.; Richardson, Alfred, Jr.; Stock, Albert M.; Tilford, C. H.; Amstutz, E. D.

CORPORATE SOURCE: Lehigh Univ., Bethlehem, PA

SOURCE: Journal of Organic Chemistry (1958), 23, 373-80
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB Pyrophthalone (I) and other 2-substituted 1,3-indandiones, R2C6H3.CO.CRR1.CO (II), their reaction products with organometallic compds., C6H4.CO.CRR1.CR2OH (III), the carbinol dehydration products, C6H4.CO.CR:CR1 (IV), and some indene, C6H4.CR1R2.CR:COH (V) and indan reduction products were prepared Chemical evidence and infrared spectra comparison showed that I and some II exist in a chelated enol form. Various methods were investigated but most II were synthesized by condensing (o-C6H4CO)2 (VI) with an alkyl heterocycle. Von Huber

[Ber. 36, 1653(1903)] heated equimolar VI and an active Me compound 5 hrs. at 200° with a catalytic amount of ZnCl2 (method A). The same procedure was used with 2 moles active Me compound in a sealed tube (method B). In the procedure of Ogilvie (U.S. 1,963,374, C.A. 28, 52519) the reactants and catalyst in PhNO2 were refluxed 6 hrs., the cooled mixture filtered, and the Et2O-washed residue recrystd. (EtNO2, PhNO2, or EtOH) (method C). In method D, o-C6H4(COCl)2 in C6H6 was used in place of VI. Method E used H3PO4 as catalyst. The phthalone in AcOH treated dropwise with 0.5 mole Br, the stirring continued 10 min., the mixture filtered and the residue slurried in H2O, the slurry made slightly basic with 5% NaOH, and the filtered residue washed and dried gave II according to method F. VI (1 mole) and 1 mole 2-methyl-benzimidazole was heated 2 hrs. at 200° according to van Alphen (C.A. 34, 50805), the product washed (hot water and AcOH) until the washings were clear, the product taken up in concentrated H2SO4, and repptd. with H2O (method G). The reactive H atoms were usually restricted to those in a Me group and the most reactive groups were those adjacent to the heterocyclic N. No product was formed by reaction of 2 Me groups. The methods of synthesis and physical data are tabulated for II (R, R1, R2, method of preparation, % yield, and m.p. given): 2-C5H4N, H, H (I), A, 7.2, 289-91°, B, 39.9, 290-2°, C, 43.1, 285-90°, D, 18, 287-90°, E, 28, 288-91°; 6,2-MeC5H3N, H, H, C, 12, 218-19°; 5,2-EtC5H3N, H, H, A, 31, 235-7°, C, 21, 235-7°; 2-C5H4N, Br, H, F, -, 152-4°; 3,2-MeC5H3N, H, H, C, 2.1, 178-80°; 4,2-MeC5H3N, H, H, C, 11, 259-60°; 2-C5H4N, Me, H, D, 15, 137-8°; 2-C5H4N, H, 4-NO2, C, 3.2, 315-16°; 6,2-MeC5H3N, H, 4-NO2, A, 14, 293-4°; 2-C5H4N, H, 5-NO2, A, 17, 352-5°; 2-C5H4N, Ph, H (VII), D, 52, 152-3°; 2-C5H5N, H, H (VIII), C, 42, 241-2°; 2-benzothiazolyl, H, H (IX), A, 51, 350-60°; 2-(5-chlorobenzimidazolyl), H, H (X), C, 61, above 480°; 2-benzimidazolyl, H, H (XI), G, 67, above 500°. Little success was had in the preparation of N-substituted pyrophthalones. For reduction of II, organolithium compds. were prepared from the appropriate halide with a molar ratio of 4:2:1 Li-organic halide-II. Finely divided Li in 35 parts by weight absolute Et2O was stirred under gentle reflux with controlled addition of 0.5M halide in Et2O, the mixture gently refluxed with controlled addition of finely powdered II, stirred under reflux to neg. Gilman test, chilled (ice-bath) and stirred with slow addition of an equal volume of dilute aqueous NH4Cl, the mixture stirred 30 min. and filtered, the solid III washed with water, and dried (method H). PhCH2MgCl (4 moles) prepared according to Gilman and Meyers [Organic Syntheses 4, 59(1925)] was refluxed 1 hr. with addition of 1 mole II and the mixture worked up as in method H (method I). III dehydrated readily and purification for characterization was difficult. Methods and data for III are tabulated (reactant, R, R1, R2, method of preparation, % yield, and m.p. given): I, 2-C5H4N, H, Ph (XII), H, 80, 142-3°; I, 2-C5H4N, H, p-MeOC6H4 (XIII), H, 70, 156-7°; I, 2-C5H4N, H, p-MeC6H4 (XIV), H, 92, 150°; I 2-C5H4N, H, m-MeC6H4 (XV), H, 75, 130°; I, 2-C5H4N, H, o-MeC6H4 (XVI), H, 70, 145-55°; I, 2-C5H4N, H, p-ClC6H4 (XVII), H, 80, 150-60°; VIII, 2-C9H6N, H, Ph (XVIII), H, 100, 164°; IX, 2-benzothiazolyl, H, Ph (XIX), H, 89, above 360°; X, 2-(5-chlorobenzimidazolyl), H, Ph, H, 49, above 510°; I, 2-C5H4N, H, PhCH2 (XX), I, 68, 100-20°; XI, 2-benzimidazolyl, H, Ph (XXI), J, 94, 235°. Also prepared were (reactant, product, method, % yield, and m.p. given): 2-indanone, 2-(2-pyridyl)-2-indanol, H, 10, 119-20°; 1-indanone,

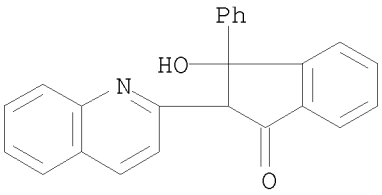
1-(2-pyridyl)-1-indanol, H, 33, 78-80°;
3-phenyl-2-(2-pyridyl)indenone (XXII),
1,3-diphenyl-2-(2-pyridyl)1-inden-3-ol (XXIII), H (the phthalone in C6H6
added to PhLi in Et2O, the mixture treated with dilute HCl and the product
crystallized from HCl), 78, 237-8°; VII,
1,2,3-triphenyl-2-(2-pyridyl)-1,3-indandiol (XXIV), H, 90, 107°.
In the reaction with XXII and VII a 2nd mole of PhLi added with formation
of XXIII and XXIV. The dried III prepared by method H or I were either
heated above the m.p. until effervesence ceased and the uniformly colored
melt recrystd. (method J) or taken up in concentrated HCl with effervescence,
the red solution stirred 15 min. at 0°, neutralized with aqueous NaOH, the
compound, washed (10% aqueous NaHCO3) and the dried material crystallized
(method K)
to give the indenones IV (reactant, R, R1, method, % yield, and m.p.
given): XII, 2-C5H4N, Ph, J, 100, 130-1°, K, 82, 129-31°;
XIII, 2-C5H4N, p-MeOC6H4 (XXV), J, 100, 155-6°; XIV, 2-C5H4N,
p-MeC6H4 (XXVI), J, 100°, 155-6°; XV, 2-C5H4N, m-MeC6H4
(XXVII), J, 100, 107-10°; XVI, 2-C5H4N, o-MeC6H4, J, 100,
121-2°; XVII, 2-C5H4N, p-ClC6H4 (XXVIII), J, 100, 136-8°;
XVIII, 2-C9H6N, Ph (XXIX), K, 96, 220°; XIX, 2-benzothiazolyl, Ph
(XXX), K, 100, 169-70°; XX, 2-C5H4N, PhCH2, K, 54, 65-100°
(gum); XXI, 2-benzimidazolyl, Ph, K, 100, 255-7°. III and IV were
unable to enolize to form chelates so that picrates, oximes, and
occasionally 2,4-dinitrophenylhydrazones were obtained. Reductions were
carried out catalytically with PtO2 or Raney Ni catalysts (method L),
according to Clemmensen (method M), and with NaBH4 method N). Vigorous
catalytic hydrogenation not only reduced indene double bonds but
occasionally reduced part or all of the heterocyclic ring substituent.
XXII (5.7 g.) in 250 absolute alc. hydrogenated 78 hrs. at 2 atmospheric with
0.2 g.
Raney Ni W-6 gave 60% V (R = 2-C5H4N, R1 = H, R2 = Ph) (XXXI), m.
188-9°. XXII (10 g.) in 30 ml. dioxane hydrogenated 16 hrs. at 2
atmospheric with 2.0 g. Raney Ni gave 10% alc.-insol. product, m. 148-9°,
and 30% XXXI, also produced in 49% yield by method N. Similar reductions
gave V (reactant, R, R1, R2, method, % yield, and m.p. given): XXII,
2-(3,4,5,6-tetrahydropyridyl), H, Ph, L, 46, 212-13°; XXIX,
2-(3,4-dihydroquinolyl), H, Ph, N, 86°, 275°; IX,
2-benzothiazolyl, H, HO, N, 100, 345-8°; XXX, 2-benzothiazolyl, H,
Ph, N, 50, 151-2°; XXVI, 2-dihydropyridyl, H, p-MeC6H4, N, 43,
183-4°. VII (1 mole), 598 g. mossy Zn, 47.9 g. HgCl2, 30 ml.
concentrated HCl, and 720 ml. H2O shaken vigorously 10 min., the residue after
decanting treated with 450 ml. H2O, 598 ml. concentrated HCl, and 1 mole VII,
the oily mixture treated with 450 ml. H2O and 598 ml. concentrated HCl, the
mixture
treated 5 times at hourly intervals with 59.8 ml. concentrated HCl and refluxed
17 hrs., the cooled solution filtered, the residue basified with NaOH, and
the water-washed product recrystd. (alc. or EtNO2) yielded 60%
2-phenyl-2-(2-pyridyl)-3-indan-1-ol, m. 186-7°. XXII was not
reduced by method M. XXII (3.3 g.) in 30 ml. absolute alc. containing 3 molar
equivs. dry HCl hydrogenated 24 hrs. at 2100 lb./sq. in. with 20 mg. PtO2
gave 15% 3-phenyl-2-(2-piperidyl)-1,3-indandiol, m. 135-6°. I (6
g.) in 50 ml. MeOH and 2.7 ml. concentrated HCl hydrogenated at 60 lb./sq. in.
over 0.5 g. PtO2 gave 11% 2-(2-piperidyl)-1,3-indandiol; HCl salt, m.
230-2° (decomposition). VII (2 g.) in 50 ml 80% AcOH hydrogenated over
PtO2 yielded 8% 2-phenyl-2-(2-piperidyl)-1,3-indandiol, m. 184-6°;
2 hrs. hydrogenation of 7.5 g. I in 100 ml. AcOH over 0.8 g. PtO2 gave 41%
2-(2-piperidyl)-1,3-hexahydroindandiol. Extensive pharmacol. screening

showed 6 indenones, XXII, XXV, XXVI, XXVII, XXVIII, XXIX, and the carbinol XIII, precursor to the indenone XXV, to have antiarthritic activity.

IT 102543-48-6P, 1-Indanone, 3-hydroxy-3-phenyl-2-(2-quinolyl)-
RL: PREP (Preparation)
(preparation of)

RN 102543-48-6 CA

CN 1H-Inden-1-one, 2,3-dihydro-3-hydroxy-3-phenyl-2-(2-quinolinyl)- (CA INDEX NAME)

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L4           0 S L2 SAM
L5           2 S L1 FULL
L6          12 S L2 FULL

     FILE 'CA' ENTERED AT 10:03:43 ON 11 FEB 2009
L7           8 S L5 OR L6

=> s organic pigment crystal?
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        161921 PIGMENT
       1956108 CRYSTAL?
L8           2 ORGANIC PIGMENT CRYSTAL?
                (ORGANIC(W)PIGMENT(W)CRYSTAL?)

=> d kwic

L8   ANSWER 1 OF 2  CA  COPYRIGHT 2009 ACS on STN
TI   Manufacture of organic pigment crystals with
     high purity and good controllability of crystal structures


=> d 2 kwic

L8   ANSWER 2 OF 2  CA  COPYRIGHT 2009 ACS on STN
TI   Fractal analysis of organic pigment crystals


=> s pigment cryst? proce?
        161921 PIGMENT
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       2272187 CRYST?
       4981145 PROCE?
L9           0 PIGMENT CRYST? PROCE?
                (PIGMENT(W)CRYST?(W)PROCE?)

=> s pigment cryst?
        161921 PIGMENT
       2272187 CRYST?
L10        289 PIGMENT CRYST?
                (PIGMENT(W)CRYST?)

=> d l8 ibib abs

L8   ANSWER 1 OF 2  CA  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        139:8131  CA
TITLE:                   Manufacture of organic pigment
                         crystals with high purity and good
                         controllability of crystal structures
INVENTOR(S):             Mizuguchi, Hitoshi
PATENT ASSIGNEE(S):      Mitsubishi Chemical Corp., Japan
SOURCE:                  Jpn. Kokai Tokkyo Koho, 8 pp.
                         CODEN: JKXXAF
DOCUMENT TYPE:           Patent
LANGUAGE:                Japanese
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    --------------------   --------
     JP 2003160738        A     20030606    JP 2001-362469         20011128
PRIORITY APPLN. INFO.:                      JP 2001-362469         20011128
AB   The manufacturing method contains heat-dissolving organic pigments in solvents
     under pressure and slowly cooling for crystallization  Thus, titanyl
     phthalocyanine, 1-chloronaphthalene, and H2O were sealed in a reactor,
     heated at 180° for 10 min, and cooled to 60° at a rate of
     3°/h to give crystals with dimensions of 200 + 400 +
     150 μm.  The pigments are useful for electroluminescence devices,
     electrophotog. toners, etc.


=> d his

     (FILE 'HOME' ENTERED AT 10:02:19 ON 11 FEB 2009)

     FILE 'REGISTRY' ENTERED AT 10:02:26 ON 11 FEB 2009
L1             STRUCTURE UPLOADED
L2             STRUCTURE UPLOADED
L3           0 S L1 SAM
L4           0 S L2 SAM
L5           2 S L1 FULL
L6          12 S L2 FULL

     FILE 'CA' ENTERED AT 10:03:43 ON 11 FEB 2009
L7           8 S L5 OR L6
L8           2 S ORGANIC PIGMENT CRYSTAL?
L9           0 S PIGMENT CRYST? PROCE?
L10        289 S PIGMENT CRYST?
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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

STN INTERNATIONAL LOGOFF AT 10:06:18 ON 11 FEB 2009